

WHAT IS CLAIMED IS:

1. A method of compressing mass spectrometry data,
comprising the steps of:
 - (a) reading data corresponding to a spectrum;
 - 5 (b) carrying out a statistical analysis of noise
within the read data to obtain at least one statistical
moment or parameter related to the distribution of that
noise;
 - (c) determining a threshold value from the, or at
10 least one of the, obtained statistical parameters;
 - (d) identifying peaks in the spectrum by comparison of
the data points in the spectrum to the said threshold value;
and
 - (e) storing information related to the identified
15 peaks along with the obtained statistical parameters.
2. The method of claim 1, wherein the step of storing
the information related to the identified peak(s) comprises
storing the data points of any peaks and discarding the
20 noise data.
3. The method of claim 1 or claim 2, further
comprising generating a mass spectrum subsequent to the step
(e) of storage.

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4. The method of claim 3, further comprising displaying the mass spectrum.

5 5. The method of claim 4, wherein the step of displaying comprises displaying only the identified peaks without also displaying the noise in the read data.

6. The method of any preceding claim, further
10 comprising, after the step of storage, reconstructing the noise data based upon one or more of the stored statistical parameters.

7. The method of claim 6 when dependent upon claim 3
15 or claim 4, wherein the step of generating the mass spectrum comprises generating the mass spectrum comprises generating a mass spectrum which includes both peak data and noise data, by combining the stored peak data with the reconstructed noise data.

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8. The method of any preceding claim, wherein the statistical moment is selected from the list comprising an expectation value, a standard deviation, and a variance.

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9. The method of claim 8, wherein the threshold is $EN+x.DN$, where EN is the expectation value and DN is the standard deviation, and wherein x is a multiplication factor.

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10. The method of claim 9, wherein x is about 2.5.

11. The method of any preceding claim, wherein the mass spectral data is FTMS data, wherein the noise in the read data is Weibull-distributed, and wherein step (b) of statistically analysing comprises identifying at least one statistical moment of the read data which best fits that Weibull distribution.

12. The method of any one of claims 1 to 10, wherein the mass spectrometric data is time of flight mass spectrometer (TOF MS) data, wherein the noise in the read data is Poisson-distributed, and wherein the step (b) of statistical analysis comprises identifying at least one statistical moment of the read data which best fits that Poisson distribution.

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13. The method of any preceding claim, wherein the step (b) of carrying out a statistical analysis of the noise comprises:

- (f) obtaining a best fit of the read data to a
5 predetermined distribution;
- (g) determining, from that best fit, one or more preliminary statistical moment(s);
- (h) generating a preliminary threshold based on the, or at least one of the, preliminary statistical moment(s);
- 10 (j) removing from the read data, all data points above that preliminary threshold; and
- (k) re-calculating a best fit of that truncated read data to a predetermined distribution so as to obtain the said at least one statistical moment or parameter related to
15 that noise in step (b).

14. The method of claim 13, further comprising:

- recursively repeating the step (j) of removing read data above a previously determined threshold, and
- 20 recursively repeating the step (f) of obtaining a best fit, this time of the further truncated data to a predetermined distribution, so as to cause convergence of the or each statistical moment.

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15. A method according to any one of the preceding claims, further comprising the step of determining the position of magnitude of the centre of any identified peaks, and wherein step (e) comprises storing any centre positions
5 and magnitudes.

16. A method according to any preceding claim, wherein step (d) comprises identifying any peaks by recognising strings of three or more consecutive data points greater
10 than the threshold.

17. A method according to any preceding claim, comprising the steps of determining the positions of two or more identified peaks, comparing the positions to determine
15 whether they are part of any predetermined isotopic sequence and, if they are, storing data points at positions corresponding to other expected peaks within the isotopic sequence.

20 18. A method according to any of claims 1 to 16, comprising the steps of determining the position of any unidentified peaks, comparing any peaks to determine any matches to predetermined parent/fragment molecular masses and, if any matches are found, storing data points

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corresponding to other expected peaks within the parent/fragment group.

19. A method of compressing mass spectrometric data,
5 comprising the steps of:

(l) reading data corresponding to a spectrum;

(m) dividing the received data into at least two
blocks;

(n) carrying out a statistical analysis on a first of
10 the at least two blocks, of noise within read data within
that block, to obtain at least one statistical moment or
parameter relating to the distribution of the noise in that
block;

(p) determining a threshold value from the, or at
15 least one of the, statistical parameters obtained in respect
of the noise within that block;

(q) identifying peaks in that block of the spectrum,
by comparison of the data points in that block of the
spectrum to the said threshold value determined for that
20 block; and

(r) storing information related to the identified
peaks in that block, along with the obtained statistical
parameters for that block.

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20. The method of claim 19, further comprising repeating steps (n) to (r) for at least one further block.

21. The method of claim 20, further comprising
5 identifying, from the plurality of blocks, a preferred block upon which the steps (n) to (q), or (n) to (r), are first to be carried out.

22. The method of claim 21, wherein the step of
10 identifying a preferred block is based upon the relative likelihood of data in a particular block having a small number of peaks in it.

23. The method of any of claims 19 to 22, wherein the
15 step (n) comprises obtaining a best fit of the read data for that block to a predetermined distribution;

determining, from that best fit, one or more preliminary statistical moment(s) for that block;

generating a preliminary threshold, based on the, or at
20 least one of the, preliminary statistical moment(s) for that block;

removing, from the read data for that block, all data points above that preliminary threshold; and

re-calculating a best fit of that truncated read data to a predetermined distribution, for that block, so as to obtain the said at least one statistical moment or parameter related to that noise in step (n) for that block.

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24. The method of claim 23, further comprising recursively repeating the step of removing data above a previously determined threshold for a particular block, and best fitting the further truncated data to a predetermined distribution, so as to cause convergence of the, or at least one of the, statistical moment(s) for that block.

25. The method of claim 23 or claim 24, further comprising repeating steps (n) to (r) of claim 19 for a next block, and wherein the step (n) further comprises, for that next block, removing, from the read data for that next block, all data points above the threshold determined for the previous block; and

re-calculating a best fit of the truncated read data in that next block to a predetermined distribution, so as to obtain a further statistical moment or moments for that next block.

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26. A mass spectrum when generated from data when compressed in accordance with the method of any one of the preceding claims.

5 27. Compressed data produced in accordance with the method of any one of the preceding claims.

28. A computer-readable medium having recorded thereon compressed mass spectrometric data generated in accordance
10 with the method of any of claims 1 to 25.

29. A method of compressing mass spectrometry data substantially as described herein with reference to any of the accompanying Figures